

Reporting Summary

Nature Research wishes to improve the reproducibility of the work that we publish. This form provides structure for consistency and transparency in reporting. For further information on Nature Research policies, see [Authors & Referees](#) and the [Editorial Policy Checklist](#).

Statistics

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.

- | | |
|-------------------------------------|---|
| n/a | Confirmed |
| ☐ | ☒ The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement |
| ☐ | ☒ A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly |
| ☒ | ☐ The statistical test(s) used AND whether they are one- or two-sided
<i>Only common tests should be described solely by name; describe more complex techniques in the Methods section.</i> |
| ☒ | ☐ A description of all covariates tested |
| ☒ | ☐ A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons |
| ☒ | ☐ A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals) |
| ☒ | ☐ For null hypothesis testing, the test statistic (e.g. F , t , r) with confidence intervals, effect sizes, degrees of freedom and P value noted
<i>Give P values as exact values whenever suitable.</i> |
| ☒ | ☐ For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings |
| ☒ | ☐ For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes |
| ☒ | ☐ Estimates of effect sizes (e.g. Cohen's d , Pearson's r), indicating how they were calculated |

Our web collection on [statistics for biologists](#) contains articles on many of the points above.

Software and code

Policy information about [availability of computer code](#)

Data collection	XDS
Data analysis	Phenix, Coot, , PyMOL, MolProbity, Autodock4, Phaser-MR, ORCA 4.0, GoodVibes 2.0.3, Gaussian 16, NBO 6.0, Bruker SHELXTL (version 2018/3), CrysAlisPro

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors/reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Research [guidelines for submitting code & software](#) for further information.

Data

Policy information about [availability of data](#)

All manuscripts must include a [data availability statement](#). This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A list of figures that have associated raw data
- A description of any restrictions on data availability

Coordinates and associated structure factors have been deposited in Protein Data Bank (PDB) with the PDB ID 6U9I (BvnE) and in the Cambridge Crystallographic Data Centre (CCDC) with the CCDC numbers 1973959 (BX), 1973957 (BY), and 1973958 (15). Sequence data referenced in this study are available in GenBank with the accession number MN401751.

Field-specific reporting

Please select the one below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.

☒ Life sciences ☐ Behavioural & social sciences ☐ Ecological, evolutionary & environmental sciences

For a reference copy of the document with all sections, see [nature.com/documents/nr-reporting-summary-flat.pdf](https://www.nature.com/documents/nr-reporting-summary-flat.pdf)

Life sciences study design

All studies must disclose on these points even when the disclosure is negative.

Sample size	For X-ray structures, sample size (total number of reflections) was determined by examining % completeness, multiplicity, and Rmerge. This typically amounted to a 360 degree rotation of a single crystal during X-ray data collection. No datasets were reported from multiple crystals. Resolution cutoffs were determined by examining I/sigma, CC1/2, and Rmerge. A thorough conformational analysis (automated with a python script for ground states and performed manually for transition states) was carried out in all the reaction steps studied computationally. Enzymatic assays were performed in triplicate.
Data exclusions	Some reflections are automatically rejected during X-ray data processing and scaling. Default rejection criteria were used in the data processing software (XDS). 5-10% of unique reflections were randomly excluded (Free-R).
Replication	All attempts at replication were successful. It should be noted that each crystal structure reported in this work was determined from a single crystal.
Randomization	Free-R flag for crystallographic data was assigned randomly to unique reflections using CCP4 program Freerflag or Phenix.
Blinding	Not applicable.

Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

Materials & experimental systems

n/a	Involved in the study
☒	☐ Antibodies
☐	☒ Eukaryotic cell lines
☒	☐ Palaeontology
☒	☐ Animals and other organisms
☒	☐ Human research participants
☒	☐ Clinical data

Methods

n/a	Involved in the study
☒	☐ ChIP-seq
☒	☐ Flow cytometry
☒	☐ MRI-based neuroimaging

Eukaryotic cell lines

Policy information about [cell lines](#)

Cell line source(s)	NRRL (Penicillium brevicompactum) & Gift from Prof. Oikawa laboratory (Aspergillus oryzae)
Authentication	Genome sequencing (Penicillium brevicompactum) & nutritional deficiency traits (Aspergillus oryzae)
Mycoplasma contamination	Negative
Commonly misidentified lines (See ICLAC register)	N/A